Full wwPDB X-ray Structure Validation Report (i)

Jul 7, 2016 – 08:07 PM EDT

PDB ID	:	4X23
Title	:	CRYSTAL STRUCTURE OF CENP-C IN COMPLEX WITH THE NUCLEOSOME CORE PARTICLE
Authors	:	Jiang, J.S.
Deposited on	:	2014-11-25
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

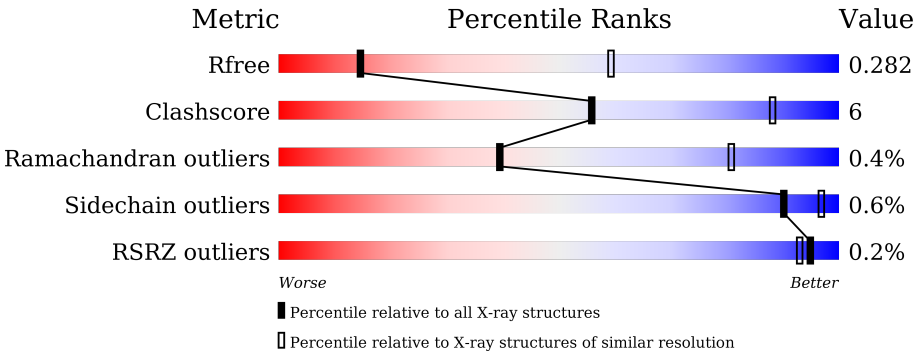
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	I	147	74% 25%
1	S	147	78% 22%
2	J	147	75% 24%
2	T	147	77% 22%
3	A	98	80% 17%
3	E	98	85% 14%

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Mol	Chain	Length	Quality of chain
3	K	98	83% 14%
3	O	98	% 81% 19%
4	B	79	81% 19%
4	F	79	% 77% 23%
4	L	79	76% 24%
4	P	79	76% 23%
5	C	102	77% 23%
5	G	102	88% 12%
5	M	102	82% 18%
5	Q	102	% 81% 19%
6	D	90	82% 18%
6	H	90	84% 16%
6	N	90	82% 18%
6	R	90	% 83% 14%
7	U	25	16% 80%
7	V	25	44% 36% 8% 12%
7	W	25	8% 88%
7	X	25	52% 32% 16%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23974 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	146	Total	C	N	O	P	0	0	0
			2975	1413	540	876	146			
1	S	146	Total	C	N	O	P	0	0	0
			2975	1413	540	876	146			

- Molecule 2 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	146	Total	C	N	O	P	0	0	0
			3011	1425	564	876	146			
2	T	146	Total	C	N	O	P	0	0	0
			3011	1425	564	876	146			

- Molecule 3 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	95	Total	C	N	O	S	0	0	0
			775	491	145	136	3			
3	E	98	Total	C	N	O	S	0	0	0
			797	504	151	139	3			
3	K	95	Total	C	N	O	S	0	0	0
			759	482	142	132	3			
3	O	98	Total	C	N	O	S	0	0	0
			791	501	148	139	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	133	ILE	-	expression tag	UNP P02299
A	134	GLU	-	expression tag	UNP P02299
A	135	GLY	-	expression tag	UNP P02299
A	136	GLY	-	expression tag	UNP P02299

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Chain	Residue	Modelled	Actual	Comment	Reference
A	137	LEU	-	expression tag	UNP P02299
E	133	ILE	-	expression tag	UNP P02299
E	134	GLU	-	expression tag	UNP P02299
E	135	GLY	-	expression tag	UNP P02299
E	136	GLY	-	expression tag	UNP P02299
E	137	LEU	-	expression tag	UNP P02299
K	133	ILE	-	expression tag	UNP P02299
K	134	GLU	-	expression tag	UNP P02299
K	135	GLY	-	expression tag	UNP P02299
K	136	GLY	-	expression tag	UNP P02299
K	137	LEU	-	expression tag	UNP P02299
O	133	ILE	-	expression tag	UNP P02299
O	134	GLU	-	expression tag	UNP P02299
O	135	GLY	-	expression tag	UNP P02299
O	136	GLY	-	expression tag	UNP P02299
O	137	LEU	-	expression tag	UNP P02299

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	79	Total	C	N	O	S	0	0	0
			622	392	120	109	1			
4	F	79	Total	C	N	O	S	0	0	0
			626	395	121	109	1			
4	L	79	Total	C	N	O	S	0	0	0
			626	395	121	109	1			
4	P	79	Total	C	N	O	S	0	0	0
			626	395	121	109	1			

- Molecule 5 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	102	Total	C	N	O	S	0	0	0
			780	491	151	137	1			
5	G	102	Total	C	N	O	S	12	0	0
			776	489	151	135	1			
5	M	102	Total	C	N	O	S	12	0	0
			780	491	151	137	1			
5	Q	102	Total	C	N	O	S	11	0	0
			780	491	151	137	1			

- Molecule 6 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	90	Total	C	N	O	S	0	0	0
			703	444	123	134	2			
6	H	90	Total	C	N	O	S	3	0	0
			703	444	123	134	2			
6	N	90	Total	C	N	O	S	3	0	0
			703	444	123	134	2			
6	R	88	Total	C	N	O	S	0	0	0
			691	438	121	130	2			

- Molecule 7 is a protein called CENP-C.

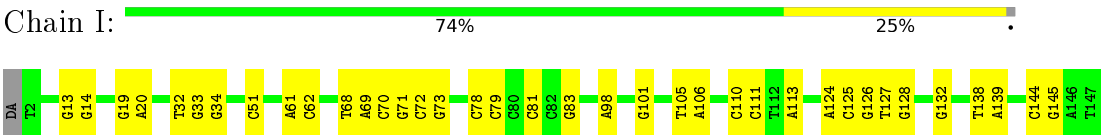
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	V	22	Total	C	N	O	0	0	0
			203	128	43	32			
7	U	5	Total	C	N	O	0	0	0
			40	24	11	5			
7	X	21	Total	C	N	O	0	0	0
			196	123	42	31			
7	W	3	Total	C	N	O	0	0	0
			25	13	7	5			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

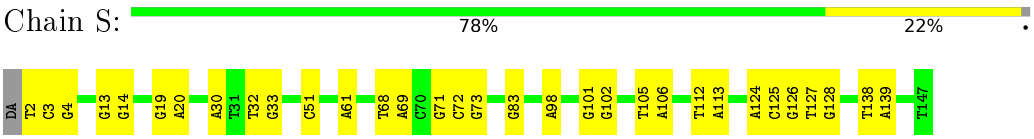
- Molecule 1: DNA (147-MER)

Chain I:



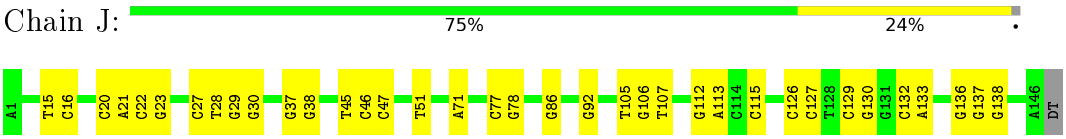
- Molecule 1: DNA (147-MER)

Chain S:



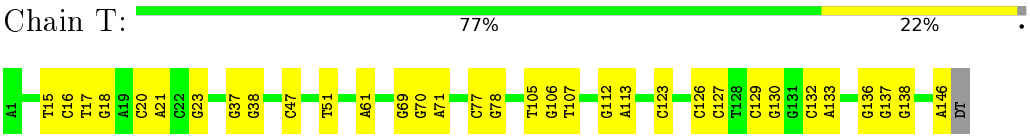
- Molecule 2: DNA (147-MER)

Chain J:



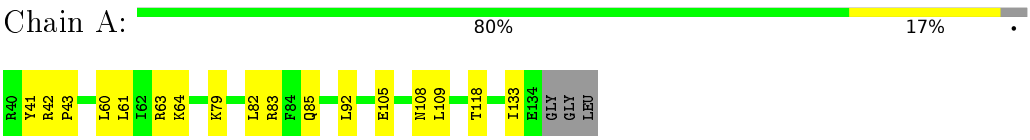
- Molecule 2: DNA (147-MER)

Chain T:



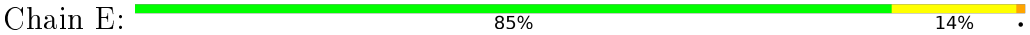
- Molecule 3: Histone H3

Chain A:

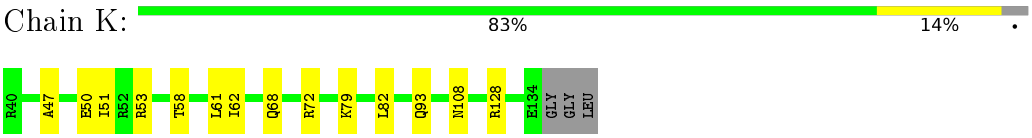


- Molecule 3: Histone H3

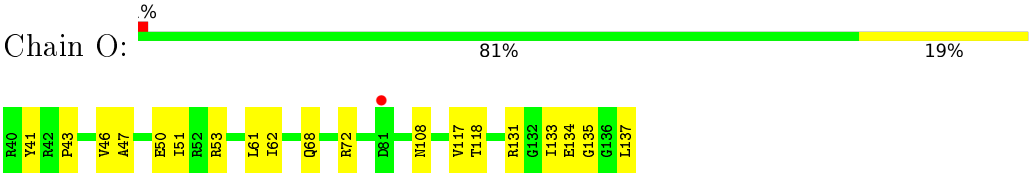
Chain E:



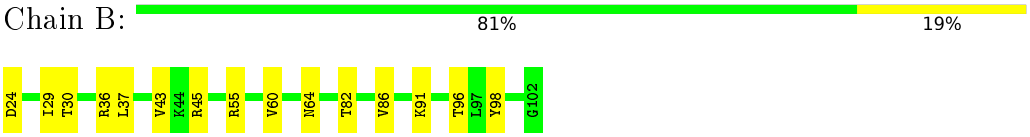
• Molecule 3: Histone H3



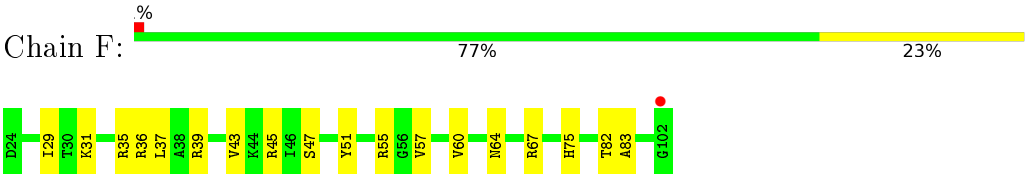
• Molecule 3: Histone H3



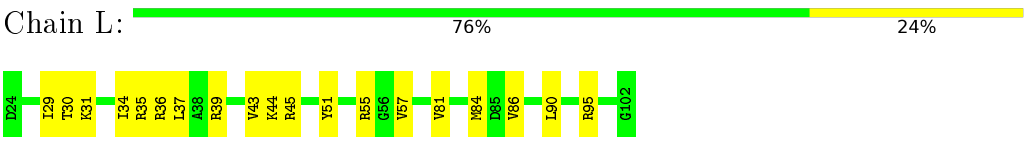
• Molecule 4: Histone H4



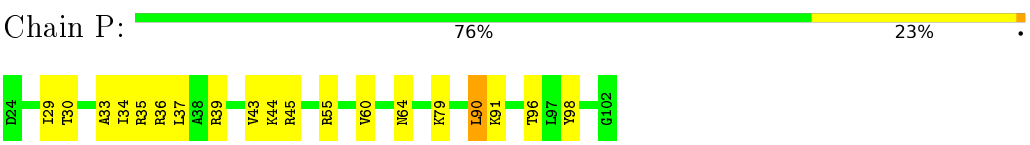
• Molecule 4: Histone H4



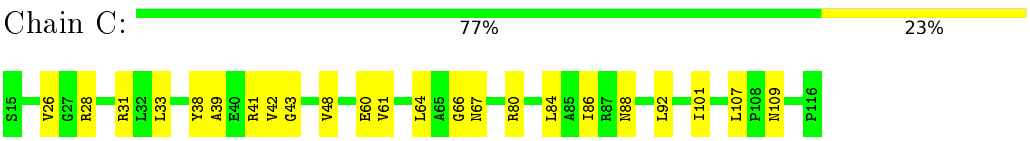
• Molecule 4: Histone H4



• Molecule 4: Histone H4

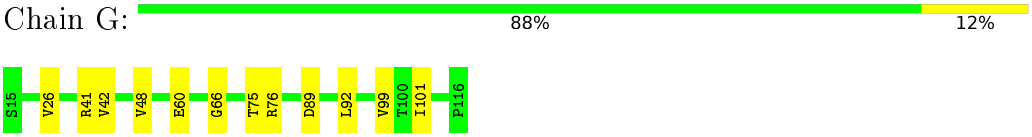


• Molecule 5: Histone H2A



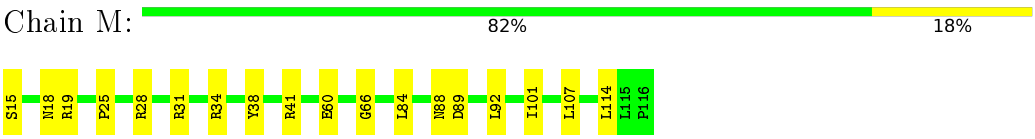
• Molecule 5: Histone H2A

Chain G:



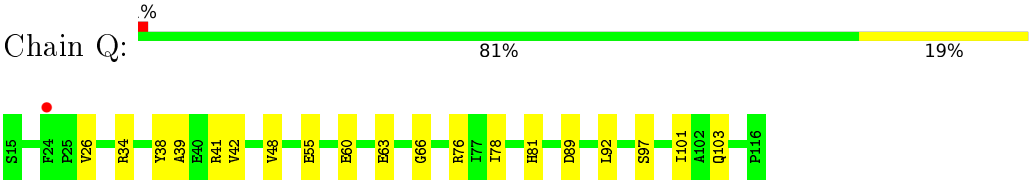
• Molecule 5: Histone H2A

Chain M:



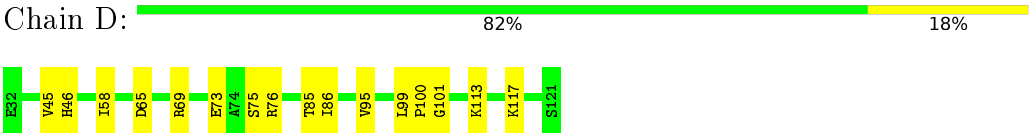
• Molecule 5: Histone H2A

Chain Q:



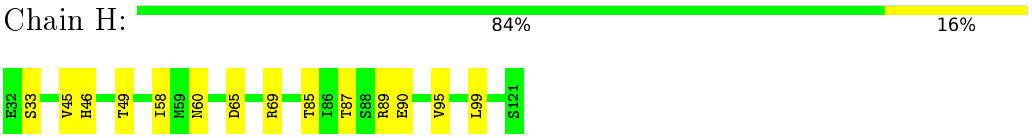
• Molecule 6: Histone H2B

Chain D:



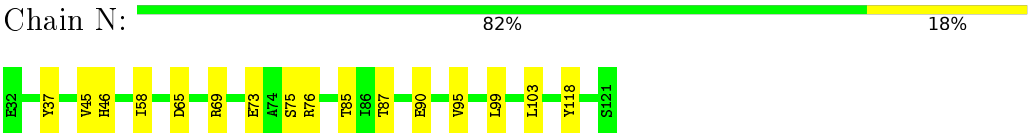
• Molecule 6: Histone H2B

Chain H:



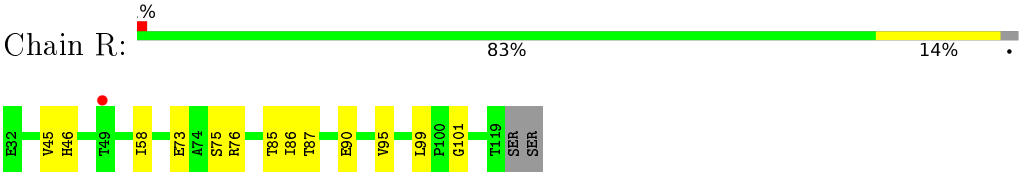
• Molecule 6: Histone H2B

Chain N:



• Molecule 6: Histone H2B

Chain R:



• Molecule 7: CENP-C

Chain V:

• Molecule 7: CENP-C

Chain U:

• Molecule 7: CENP-C

Chain X:

• Molecule 7: CENP-C

Chain W:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.99Å 176.10Å 208.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.54 – 3.50 49.54 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.54-3.50) 92.1 (49.54-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1690)	Depositor
R, R_{free}	0.236 , 0.286 0.235 , 0.282	Depositor DCC
R_{free} test set	1718 reflections (3.77%)	DCC
Wilson B-factor (Å^2)	111.6	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 75.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	23974	wwPDB-VP
Average B, all atoms (Å^2)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	I	0.49	0/3333	0.88	0/5137
1	S	0.49	0/3333	0.88	0/5137
2	J	0.50	0/3381	0.87	0/5221
2	T	0.50	0/3381	0.87	0/5221
3	A	0.20	0/785	0.39	0/1054
3	E	0.20	0/807	0.36	0/1082
3	K	0.20	0/769	0.36	0/1034
3	O	0.20	0/801	0.36	0/1075
4	B	0.20	0/629	0.37	0/844
4	F	0.20	0/633	0.37	0/848
4	L	0.20	0/633	0.38	0/848
4	P	0.20	0/633	0.37	0/848
5	C	0.20	0/790	0.42	0/1068
5	G	0.19	0/786	0.36	0/1063
5	M	0.20	0/790	0.35	0/1068
5	Q	0.20	0/790	0.36	0/1068
6	D	0.20	0/714	0.37	0/963
6	H	0.21	0/714	0.37	0/963
6	N	0.21	0/714	0.38	0/963
6	R	0.21	0/702	0.40	0/947
7	U	0.17	0/39	0.32	0/50
7	V	0.23	0/207	0.53	0/276
7	W	0.18	0/24	0.30	0/30
7	X	0.25	0/200	0.56	0/266
All	All	0.38	0/25588	0.70	0/37074

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2975	0	1639	27	0
1	S	2975	0	1639	24	0
2	J	3011	0	1639	28	0
2	T	3011	0	1639	27	0
3	A	775	0	811	14	0
3	E	797	0	839	14	0
3	K	759	0	785	12	0
3	O	791	0	828	17	0
4	B	622	0	652	12	0
4	F	626	0	663	13	0
4	L	626	0	663	13	0
4	P	626	0	663	18	0
5	C	780	0	822	16	0
5	G	776	0	818	11	0
5	M	780	0	822	18	0
5	Q	780	0	822	17	0
6	D	703	0	720	11	0
6	H	703	0	720	11	0
6	N	703	0	720	15	0
6	R	691	0	710	10	0
7	U	40	0	40	1	0
7	V	203	0	208	9	0
7	W	25	0	23	2	0
7	X	196	0	199	7	0
All	All	23974	0	19084	246	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (246) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:60:GLU:OE2	7:W:717:ARG:HD2	1.63	0.99
5:M:60:GLU:OE2	7:W:717:ARG:CD	2.24	0.86
4:P:29:ILE:HD11	4:P:55:ARG:HG2	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:729:GLU:HG3	7:X:733:TYR:HB2	1.71	0.72
4:F:29:ILE:HD11	4:F:55:ARG:HG2	1.72	0.71
4:B:29:ILE:HD11	4:B:55:ARG:HG2	1.73	0.71
5:Q:63:GLU:OE2	7:X:719:ARG:NH2	2.25	0.70
4:L:29:ILE:HD11	4:L:55:ARG:HG2	1.74	0.69
7:V:733:TYR:HB2	7:X:729:GLU:HB2	1.74	0.69
5:G:66:GLY:HA3	6:H:46:HIS:HD2	1.58	0.68
2:T:51:DT:OP1	3:O:72:ARG:NH1	2.27	0.68
5:C:41:ARG:HB2	6:D:85:THR:HG22	1.75	0.67
3:E:133:ILE:HG23	3:E:137:LEU:HD13	1.75	0.67
3:K:50:GLU:HA	3:K:53:ARG:HG2	1.76	0.67
3:O:131:ARG:HB3	3:O:135:GLY:HA3	1.77	0.67
3:E:50:GLU:HA	3:E:53:ARG:HG2	1.77	0.66
5:Q:66:GLY:HA3	6:R:46:HIS:HD2	1.61	0.66
7:V:725:TYR:O	7:V:727:ARG:N	2.26	0.65
1:S:113:DA:OP1	5:Q:42:VAL:N	2.29	0.65
3:E:79:LYS:HD3	3:E:82:LEU:HD21	1.80	0.64
3:O:50:GLU:HA	3:O:53:ARG:HG2	1.78	0.64
6:H:45:VAL:O	6:H:46:HIS:ND1	2.31	0.64
1:S:126:DG:O6	2:T:21:DA:N6	2.31	0.63
2:T:71:DA:H5'	4:P:45:ARG:HH21	1.64	0.63
5:M:41:ARG:HB2	6:N:85:THR:HG22	1.80	0.63
3:O:108:ASN:HB2	4:P:43:VAL:HG12	1.81	0.62
4:P:60:VAL:O	4:P:64:ASN:ND2	2.32	0.62
5:C:39:ALA:HB2	6:D:86:ILE:HD13	1.82	0.61
6:D:45:VAL:O	6:D:46:HIS:ND1	2.34	0.61
1:I:125:DC:O2	2:J:23:DG:N2	2.30	0.61
1:S:71:DG:H5'	4:L:45:ARG:HH21	1.65	0.61
6:N:45:VAL:O	6:N:46:HIS:ND1	2.33	0.61
5:Q:89:ASP:HB3	5:Q:92:LEU:HB2	1.82	0.61
5:Q:60:GLU:OE2	7:X:719:ARG:NH1	2.34	0.61
1:I:71:DG:H5'	4:B:45:ARG:HH21	1.66	0.60
6:R:45:VAL:O	6:R:46:HIS:ND1	2.33	0.60
1:S:125:DC:O2	2:T:23:DG:N2	2.33	0.60
5:G:41:ARG:HB2	6:H:85:THR:HG22	1.83	0.60
5:Q:38:TYR:HB3	6:R:75:SER:HB2	1.85	0.59
5:C:33:LEU:HB3	5:C:42:VAL:HG11	1.85	0.59
6:D:75:SER:HA	6:D:86:ILE:HD11	1.85	0.58
3:A:60:LEU:HD12	3:A:64:LYS:HE2	1.85	0.58
3:E:125:GLN:HB3	7:V:726:TRP:HD1	1.69	0.58
5:G:60:GLU:OE2	7:V:719:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:29:ILE:HD13	4:P:34:ILE:HD11	1.85	0.58
1:S:101:DG:N2	2:T:47:DC:O2	2.28	0.58
6:D:73:GLU:OE1	6:D:76:ARG:NH2	2.34	0.57
6:D:95:VAL:HG13	6:D:99:LEU:HD23	1.86	0.57
1:S:61:DA:H5"	4:L:30:THR:HG21	1.86	0.57
5:M:66:GLY:HA3	6:N:46:HIS:HD2	1.70	0.57
3:A:85:GLN:HG3	4:B:82:THR:HA	1.87	0.57
5:C:101:ILE:HG23	6:D:58:ILE:HD13	1.86	0.57
3:O:61:LEU:HD12	4:P:37:LEU:HD23	1.87	0.57
3:K:79:LYS:HD3	3:K:82:LEU:HD21	1.87	0.57
7:V:725:TYR:C	7:V:727:ARG:H	2.08	0.57
5:C:60:GLU:OE2	7:U:719:ARG:NH2	2.37	0.57
1:I:101:DG:N2	2:J:47:DC:O2	2.31	0.56
5:Q:55:GLU:OE2	7:X:714:ARG:NH1	2.28	0.56
6:R:73:GLU:OE1	6:R:76:ARG:NH2	2.35	0.56
2:J:71:DA:H5'	4:F:45:ARG:HH21	1.70	0.56
3:E:61:LEU:HD12	4:F:37:LEU:HD23	1.86	0.55
5:M:88:ASN:HD21	5:M:107:LEU:HD21	1.72	0.55
1:S:51:DC:OP1	3:K:72:ARG:NH1	2.37	0.55
3:O:133:ILE:HG22	3:O:137:LEU:HD13	1.89	0.54
3:K:61:LEU:HD12	4:L:37:LEU:HD23	1.88	0.54
5:C:66:GLY:HA3	6:D:46:HIS:HD2	1.73	0.54
4:L:29:ILE:HD13	4:L:34:ILE:HD11	1.89	0.54
2:T:123:DC:OP1	5:M:28:ARG:NH2	2.36	0.54
5:Q:39:ALA:HB2	6:R:86:ILE:HD13	1.89	0.54
5:Q:101:ILE:HG23	6:R:58:ILE:HD13	1.90	0.53
4:B:91:LYS:HE2	4:B:96:THR:HG23	1.91	0.53
2:T:113:DA:OP2	5:M:34:ARG:NH2	2.42	0.53
2:T:20:DC:O3'	5:Q:76:ARG:NH1	2.42	0.52
4:B:60:VAL:O	4:B:64:ASN:ND2	2.38	0.52
5:G:66:GLY:HA3	6:H:46:HIS:CD2	2.43	0.52
1:S:3:DC:H4'	1:S:4:DG:OP1	2.09	0.52
4:F:60:VAL:O	4:F:64:ASN:ND2	2.39	0.52
2:J:51:DT:OP1	3:E:72:ARG:NH1	2.43	0.52
3:A:61:LEU:HD12	4:B:37:LEU:HD23	1.92	0.52
3:A:79:LYS:HB3	3:A:82:LEU:HD11	1.92	0.51
6:N:95:VAL:HG13	6:N:99:LEU:HD23	1.92	0.51
6:N:73:GLU:OE1	6:N:76:ARG:NH2	2.41	0.51
6:H:65:ASP:OD2	6:H:69:ARG:NH2	2.44	0.51
5:C:86:ILE:HA	5:C:92:LEU:HD23	1.93	0.51
3:K:68:GLN:HE21	3:K:72:ARG:HH21	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:27:DC:H2"	2:J:28:DT:C5	2.47	0.50
3:O:47:ALA:O	3:O:51:ILE:HG13	2.12	0.50
1:S:32:DT:H2"	1:S:33:DG:H5'	1.94	0.50
1:I:138:DT:H2"	1:I:139:DA:C8	2.47	0.49
5:Q:66:GLY:HA3	6:R:46:HIS:CD2	2.46	0.49
5:Q:41:ARG:HB2	6:R:85:THR:HG22	1.95	0.49
5:C:84:LEU:O	5:C:88:ASN:ND2	2.30	0.49
5:M:38:TYR:HB3	6:N:75:SER:HB2	1.94	0.49
1:I:105:DT:H2"	1:I:106:DA:O5'	2.12	0.49
1:S:138:DT:H2"	1:S:139:DA:C8	2.48	0.49
1:I:68:DT:H2"	1:I:69:DA:C8	2.48	0.49
1:S:68:DT:H2"	1:S:69:DA:C8	2.47	0.49
2:T:71:DA:OP1	3:O:117:VAL:N	2.45	0.49
1:S:105:DT:H2"	1:S:106:DA:O5'	2.12	0.49
5:C:38:TYR:HB3	6:D:75:SER:HB2	1.96	0.48
4:L:90:LEU:HB3	4:L:95:ARG:O	2.14	0.48
7:V:715:SER:OG	7:V:716:ASN:N	2.47	0.48
2:T:106:DG:H2"	2:T:107:DT:H5"	1.96	0.48
2:T:15:DT:H2"	2:T:16:DC:O5'	2.14	0.48
1:I:126:DG:O6	2:J:21:DA:N6	2.47	0.48
1:I:32:DT:H2"	1:I:33:DG:H5'	1.96	0.48
1:S:2:DT:H73	2:T:146:DA:H2	1.77	0.48
2:J:20:DC:O3'	5:G:76:ARG:NH1	2.47	0.47
7:X:715:SER:OG	7:X:716:ASN:N	2.47	0.47
4:L:86:VAL:HG23	4:L:90:LEU:HD23	1.96	0.47
5:G:75:THR:HG22	6:H:49:THR:HA	1.96	0.47
1:I:144:DC:H2"	1:I:145:DG:C8	2.50	0.47
3:O:68:GLN:OE1	3:O:72:ARG:NH2	2.47	0.47
1:S:124:DA:H1'	1:S:125:DC:H5'	1.96	0.47
3:O:133:ILE:HG12	5:Q:97:SER:HB2	1.96	0.46
2:J:112:DG:H5"	5:C:43:GLY:HA2	1.97	0.46
2:J:15:DT:H2"	2:J:16:DC:O5'	2.14	0.46
5:M:66:GLY:HA3	6:N:46:HIS:CD2	2.49	0.46
5:M:101:ILE:HG23	6:N:58:ILE:HD13	1.98	0.46
5:C:107:LEU:O	5:C:109:ASN:ND2	2.46	0.46
2:J:106:DG:H2"	2:J:107:DT:H5"	1.97	0.46
4:L:39:ARG:NH1	4:L:44:LYS:O	2.37	0.46
6:H:95:VAL:HG13	6:H:99:LEU:HD23	1.97	0.46
1:I:61:DA:H5"	4:B:30:THR:HG21	1.97	0.46
2:J:92:DG:H5'	3:A:63:ARG:HH22	1.81	0.45
5:G:101:ILE:HG23	6:H:58:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:133:ILE:HD12	3:O:134:GLU:HG2	1.97	0.45
1:I:110:DC:H2"	1:I:111:DC:C5	2.51	0.45
4:L:31:LYS:HG3	4:L:51:TYR:CE1	2.51	0.45
3:O:61:LEU:HB3	4:P:36:ARG:HG3	1.97	0.45
2:T:137:DG:H2"	2:T:138:DG:C8	2.52	0.45
5:G:26:VAL:HG11	5:G:48:VAL:HG22	1.98	0.45
1:S:98:DA:H5'	1:S:98:DA:C8	2.52	0.45
1:S:13:DG:H2"	1:S:14:DG:H5'	1.99	0.45
3:E:61:LEU:HB3	4:F:36:ARG:HG3	1.99	0.45
1:I:98:DA:H5'	1:I:98:DA:C8	2.52	0.45
4:B:98:TYR:CZ	5:G:99:VAL:HG11	2.52	0.44
6:R:95:VAL:HG13	6:R:99:LEU:HD23	2.00	0.44
4:F:75:HIS:O	6:H:89:ARG:NH1	2.38	0.44
3:A:108:ASN:HB2	4:B:43:VAL:HG12	1.99	0.44
2:J:132:DC:H2"	2:J:133:DA:C8	2.52	0.44
2:T:129:DC:H2"	2:T:130:DG:C8	2.52	0.44
1:I:113:DA:OP1	5:G:42:VAL:N	2.43	0.44
5:M:15:SER:HB3	5:M:18:ASN:HB2	1.99	0.44
6:D:113:LYS:O	6:D:117:LYS:HG3	2.18	0.44
6:D:65:ASP:O	6:D:69:ARG:HB2	2.18	0.44
4:F:35:ARG:O	4:F:39:ARG:HG2	2.17	0.44
3:K:47:ALA:O	3:K:51:ILE:HG13	2.18	0.44
1:S:72:DC:H2"	1:S:73:DG:C8	2.53	0.44
5:C:26:VAL:HG11	5:C:48:VAL:HG22	2.00	0.43
1:I:13:DG:H2"	1:I:14:DG:H5'	2.00	0.43
4:P:91:LYS:HG3	4:P:96:THR:HG23	2.00	0.43
5:M:19:ARG:HH11	6:N:118:TYR:HE1	1.66	0.43
4:P:35:ARG:O	4:P:39:ARG:HG2	2.17	0.43
3:E:125:GLN:HB3	7:V:726:TRP:CD1	2.50	0.43
3:E:41:TYR:HB3	3:E:42:ARG:H	1.57	0.43
5:M:19:ARG:HD2	6:N:118:TYR:CE1	2.53	0.43
5:C:64:LEU:HA	5:C:67:ASN:HD21	1.84	0.43
6:N:65:ASP:OD2	6:N:69:ARG:NH2	2.49	0.43
4:L:35:ARG:O	4:L:39:ARG:HG2	2.19	0.43
2:T:17:DT:H2"	2:T:18:DG:C8	2.54	0.43
2:T:37:DG:H2"	2:T:38:DG:H5'	2.01	0.43
2:J:129:DC:H2"	2:J:130:DG:C8	2.54	0.43
2:J:136:DG:H2"	2:J:137:DG:OP2	2.19	0.43
3:A:105:GLU:O	3:A:109:LEU:HD13	2.19	0.43
3:A:61:LEU:HB3	4:B:36:ARG:HG3	2.01	0.42
5:C:80:ARG:HB2	3:E:58:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:34:DG:N2	2:J:115:DC:O2	2.52	0.42
2:J:129:DC:H2"	2:J:130:DG:N7	2.34	0.42
3:K:128:ARG:NH1	4:L:57:VAL:HG12	2.34	0.42
5:M:84:LEU:O	5:M:88:ASN:ND2	2.28	0.42
2:T:112:DG:H2"	2:T:113:DA:C8	2.54	0.42
2:J:22:DC:H2"	2:J:23:DG:H8	1.84	0.42
5:C:28:ARG:O	5:C:31:ARG:HG2	2.19	0.42
2:T:129:DC:H2"	2:T:130:DG:N7	2.33	0.42
4:F:67:ARG:HH22	7:V:730:ARG:NH2	2.17	0.42
1:I:62:DC:H42	2:J:86:DG:H1	1.67	0.42
6:N:87:THR:OG1	6:N:90:GLU:OE1	2.25	0.42
3:O:118:THR:OG1	4:P:45:ARG:NE	2.50	0.42
2:J:126:DC:H2"	2:J:127:DC:OP1	2.19	0.42
2:J:29:DG:H2"	2:J:30:DG:C8	2.55	0.42
4:P:90:LEU:HA	4:P:90:LEU:HD12	1.88	0.42
3:K:58:THR:OG1	5:Q:103:GLN:O	2.35	0.42
5:Q:26:VAL:HG11	5:Q:48:VAL:HG22	1.99	0.42
2:T:15:DT:H4'	2:T:16:DC:OP1	2.20	0.42
1:S:30:DA:OP2	5:M:31:ARG:HD3	2.20	0.42
4:P:39:ARG:NH1	4:P:44:LYS:O	2.39	0.42
2:T:105:DT:H2"	2:T:106:DG:C8	2.54	0.42
3:A:41:TYR:HB3	3:A:42:ARG:H	1.67	0.42
4:F:31:LYS:HG3	4:F:51:TYR:CE1	2.54	0.42
1:I:19:DG:H2"	1:I:20:DA:C8	2.54	0.42
2:J:15:DT:H4'	2:J:16:DC:OP1	2.20	0.42
1:S:102:DG:OP1	4:P:79:LYS:N	2.52	0.42
1:S:83:DG:OP1	3:O:46:VAL:N	2.52	0.42
2:J:112:DG:H2"	2:J:113:DA:C8	2.55	0.42
2:J:77:DC:H2"	2:J:78:DG:H5'	2.01	0.42
5:M:114:LEU:HD22	4:P:44:LYS:HB2	2.02	0.42
1:S:19:DG:H2"	1:S:20:DA:C8	2.55	0.42
1:I:124:DA:H1'	1:I:125:DC:H5'	2.01	0.41
3:K:62:ILE:HD11	3:K:93:GLN:HG3	2.02	0.41
3:K:108:ASN:HB2	4:L:43:VAL:HG12	2.02	0.41
6:H:87:THR:OG1	6:H:90:GLU:OE1	2.29	0.41
6:N:58:ILE:HG23	4:P:98:TYR:HB3	2.02	0.41
6:R:87:THR:OG1	6:R:90:GLU:OE1	2.28	0.41
2:T:69:DG:H5"	3:O:43:PRO:HB2	2.03	0.41
2:T:70:DG:H4'	4:P:45:ARG:NE	2.34	0.41
3:E:42:ARG:HA	3:E:43:PRO:HD3	1.93	0.41
5:C:61:VAL:HG22	5:C:92:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:78:DC:H2"	1:I:79:DC:C5	2.55	0.41
1:I:83:DG:H5'	3:E:43:PRO:HA	2.01	0.41
2:T:77:DC:H2"	2:T:78:DG:H5'	2.02	0.41
1:I:127:DT:H2"	1:I:128:DG:C8	2.56	0.41
1:I:70:DC:H2"	1:I:71:DG:C8	2.56	0.41
2:J:37:DG:H2"	2:J:38:DG:H5'	2.03	0.41
3:A:92:LEU:HD22	4:B:86:VAL:HG11	2.03	0.41
3:O:133:ILE:HG13	3:O:133:ILE:H	1.55	0.41
3:E:108:ASN:HB2	4:F:43:VAL:HG12	2.03	0.41
2:J:137:DG:H2"	2:J:138:DG:C8	2.56	0.41
5:M:89:ASP:HB3	5:M:92:LEU:HB2	2.01	0.41
3:E:128:ARG:NH1	4:F:57:VAL:HG12	2.35	0.41
1:I:81:DC:H5"	4:F:47:SER:HA	2.02	0.41
1:I:71:DG:OP1	3:A:118:THR:N	2.51	0.41
5:M:25:PRO:HD3	6:N:37:TYR:CD2	2.56	0.41
2:T:136:DG:H2"	2:T:137:DG:OP2	2.19	0.41
3:K:61:LEU:HB3	4:L:36:ARG:HG3	2.01	0.41
3:A:42:ARG:HA	3:A:43:PRO:HD3	1.90	0.41
4:B:24:ASP:N	4:B:24:ASP:OD1	2.54	0.41
3:O:62:ILE:HG22	4:P:33:ALA:HB1	2.03	0.41
2:T:132:DC:H2"	2:T:133:DA:C8	2.56	0.41
6:H:33:SER:HB2	6:H:60:ASN:OD1	2.21	0.40
1:I:72:DC:H2"	1:I:73:DG:C8	2.57	0.40
1:S:51:DC:OP2	3:K:72:ARG:NH2	2.44	0.40
3:A:133:ILE:HG13	3:A:133:ILE:H	1.60	0.40
4:F:82:THR:OG1	4:F:83:ALA:N	2.54	0.40
1:I:132:DG:N2	2:J:16:DC:O2	2.53	0.40
5:Q:78:ILE:HG12	5:Q:81:HIS:CE1	2.55	0.40
1:S:112:DT:H2"	1:S:113:DA:C8	2.56	0.40
5:G:89:ASP:HB3	5:G:92:LEU:HB2	2.03	0.40
1:I:51:DC:H5'	3:A:83:ARG:HG2	2.04	0.40
2:J:105:DT:H2"	2:J:106:DG:C8	2.56	0.40
6:N:103:LEU:HA	6:N:103:LEU:HD23	1.89	0.40
2:J:45:DT:H2"	2:J:46:DC:H5'	2.02	0.40
2:T:61:DA:H5"	4:P:30:THR:HG21	2.04	0.40
5:Q:89:ASP:OD2	7:X:717:ARG:NH2	2.54	0.40
1:S:127:DT:H2"	1:S:128:DG:C8	2.56	0.40
2:T:126:DC:H2"	2:T:127:DC:OP1	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	93/98 (95%)	89 (96%)	4 (4%)	0	100 100
3	E	96/98 (98%)	91 (95%)	4 (4%)	1 (1%)	19 66
3	K	93/98 (95%)	89 (96%)	4 (4%)	0	100 100
3	O	96/98 (98%)	94 (98%)	2 (2%)	0	100 100
4	B	77/79 (98%)	74 (96%)	3 (4%)	0	100 100
4	F	77/79 (98%)	74 (96%)	3 (4%)	0	100 100
4	L	77/79 (98%)	74 (96%)	3 (4%)	0	100 100
4	P	77/79 (98%)	74 (96%)	3 (4%)	0	100 100
5	C	100/102 (98%)	95 (95%)	5 (5%)	0	100 100
5	G	100/102 (98%)	95 (95%)	5 (5%)	0	100 100
5	M	100/102 (98%)	95 (95%)	5 (5%)	0	100 100
5	Q	100/102 (98%)	95 (95%)	5 (5%)	0	100 100
6	D	88/90 (98%)	84 (96%)	2 (2%)	2 (2%)	8 48
6	H	88/90 (98%)	85 (97%)	3 (3%)	0	100 100
6	N	88/90 (98%)	84 (96%)	4 (4%)	0	100 100
6	R	86/90 (96%)	84 (98%)	1 (1%)	1 (1%)	16 61
7	U	3/25 (12%)	2 (67%)	1 (33%)	0	100 100
7	V	20/25 (80%)	11 (55%)	7 (35%)	2 (10%)	1 9
7	W	1/25 (4%)	1 (100%)	0	0	100 100
7	X	19/25 (76%)	12 (63%)	7 (37%)	0	100 100
All	All	1479/1576 (94%)	1402 (95%)	71 (5%)	6 (0%)	39 81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	V	726	TRP

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Mol	Chain	Res	Type
6	R	101	GLY
6	D	100	PRO
6	D	101	GLY
7	V	725	TYR
3	E	43	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	82/84 (98%)	82 (100%)	0	100	100
3	E	84/84 (100%)	84 (100%)	0	100	100
3	K	78/84 (93%)	78 (100%)	0	100	100
3	O	83/84 (99%)	82 (99%)	1 (1%)	78	92
4	B	63/64 (98%)	63 (100%)	0	100	100
4	F	64/64 (100%)	64 (100%)	0	100	100
4	L	64/64 (100%)	62 (97%)	2 (3%)	47	81
4	P	64/64 (100%)	63 (98%)	1 (2%)	70	89
5	C	79/79 (100%)	79 (100%)	0	100	100
5	G	78/79 (99%)	78 (100%)	0	100	100
5	M	79/79 (100%)	79 (100%)	0	100	100
5	Q	79/79 (100%)	78 (99%)	1 (1%)	76	91
6	D	77/77 (100%)	77 (100%)	0	100	100
6	H	77/77 (100%)	77 (100%)	0	100	100
6	N	77/77 (100%)	77 (100%)	0	100	100
6	R	75/77 (97%)	75 (100%)	0	100	100
7	U	3/24 (12%)	3 (100%)	0	100	100
7	V	21/24 (88%)	19 (90%)	2 (10%)	11	43
7	W	3/24 (12%)	3 (100%)	0	100	100
7	X	20/24 (83%)	19 (95%)	1 (5%)	30	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1250/1312 (95%)	1242 (99%)	8 (1%)	90 97

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	V	717	ARG
7	V	732	ASP
4	L	81	VAL
4	L	84	MET
3	O	41	TYR
4	P	90	LEU
5	Q	34	ARG
7	X	732	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	I	146/147 (99%)	-0.52	0 100 100	126, 188, 227, 250	0
1	S	146/147 (99%)	-0.30	0 100 100	146, 211, 254, 271	0
2	J	146/147 (99%)	-0.39	0 100 100	125, 188, 228, 241	0
2	T	146/147 (99%)	-0.28	0 100 100	161, 212, 253, 266	0
3	A	95/98 (96%)	-0.18	0 100 100	70, 109, 157, 168	0
3	E	98/98 (100%)	-0.20	0 100 100	74, 102, 143, 161	0
3	K	95/98 (96%)	-0.09	0 100 100	86, 119, 160, 175	0
3	O	98/98 (100%)	-0.04	1 (1%) 84 76	78, 127, 186, 220	0
4	B	79/79 (100%)	-0.07	0 100 100	71, 106, 146, 158	0
4	F	79/79 (100%)	-0.07	1 (1%) 79 70	75, 97, 136, 149	0
4	L	79/79 (100%)	-0.07	0 100 100	73, 112, 147, 159	0
4	P	79/79 (100%)	-0.11	0 100 100	82, 119, 150, 163	0
5	C	102/102 (100%)	-0.25	0 100 100	72, 109, 143, 167	0
5	G	102/102 (100%)	-0.18	0 100 100	73, 100, 136, 162	4 (3%)
5	M	102/102 (100%)	-0.19	0 100 100	79, 116, 154, 168	4 (3%)
5	Q	102/102 (100%)	-0.20	1 (0%) 84 76	83, 115, 158, 179	4 (3%)
6	D	90/90 (100%)	-0.23	0 100 100	79, 109, 138, 156	0
6	H	90/90 (100%)	-0.20	0 100 100	73, 102, 141, 155	1 (1%)
6	N	90/90 (100%)	-0.21	0 100 100	82, 114, 149, 159	1 (1%)
6	R	88/90 (97%)	-0.14	1 (1%) 82 73	83, 116, 149, 171	0
7	U	5/25 (20%)	-0.19	0 100 100	137, 155, 164, 178	0
7	V	22/25 (88%)	-0.14	0 100 100	86, 126, 159, 176	0
7	W	3/25 (12%)	0.06	0 100 100	159, 159, 168, 179	0
7	X	21/25 (84%)	-0.22	0 100 100	93, 135, 160, 194	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	2103/2164 (97%)	-0.22	4 (0%)	95	93	70, 124, 226, 271	14 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	81	ASP	3.2
5	Q	24	PHE	2.3
4	F	102	GLY	2.3
6	R	49	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.